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# Electronic Properties of Phosphorene/Graphene Heterostructures: Effect of External Electric Field

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**Abstract.** We report the electronic properties of electrically gated heterostructures of black and blue phosphorene with graphene. The heterostructure of blue phosphorene with graphene is energetically more favorable than black phospherene/graphene. However, both are bonded by weak interlayer interactions. Graphene induces the Dirac cone character in both heterostructure which shows tunabilities with external electric field. It is found that Dirac cone get shifted depending on the polarity of external electric field that results into the so called self induced p-type or n-type doping effect. These features have importance in the fabrication of nano-electronic devices based on the phosphorene /graphene heterostructures.

**Keywords:** Hetrostructure, Phospherene, Graphene, Schottky barrier.
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## INTRODUCTION

The successful exfoliation of graphene from the graphite crystal has stimulated the research area in 2D materials [1]. However, lack of electronic band gap in graphene limits its utilization in full potential which lead to the discovery of new class of 2D materials including layered transition metal dichalchogenides, silicene and germanene[2].

Phosphorene, a monoatomic layer of black phosphorous (black-P), has recently been included in the family of 2D materials as a promising contender for nano- and opto-electronic applications due to its novel physical and chemical properties [3]. The stable atomic layer of black-P exhibit puckered structure [4], whereas the graphene-like honeycomb structure of phosphorous namely blue phosphorous (blue-P), recently predicted, exhibits an intrinsic indirect band gap of ~2eV as compared to direct band gap of ~1eV in black-P [5.].

Vertical hetero-structuring of 2D materials is currently considered as a modernistic way to fabricate devices with desired opto- or nano-electronic properties. The combination of exotic properties of graphene with black-P by making their vertical heterostructures, for the superior nanoelectronic applications, remain the novel idea in recent investigations [6, 7]. In this paper, we present the external electric field induced changes in the electronic properties of the hetero-structures of black-P/graphene and blue-P/graphene in the framework of density functional theory (DFT).

## COMPUTATIONAL DETAILS

The first principles calculations are carried out by means of pseudo-potential and numerical atomic orbitals (NAOs) basis sets, as implemented in SIESTA package [8]. The generalized gradient approximation (GGA) in the form of Perdew-Burke-Ernzerhof (PBE) exchange correlation functional is used to treat electron-electron interactions. Structural optimizations are performed using conjugate gradient method until the residual forces on each atom is less than 0.01 eV/Å. Double zeta polarization (DZP) basis sets are used to expand the Kohn-Sham orbitals with meshcutoff energy of 200 Ry. The Brillouin zone was sampled using Monkhorst-pack scheme with a 10×10×1 mesh for calculations.

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## RESULTS AND DISCUSSIONS

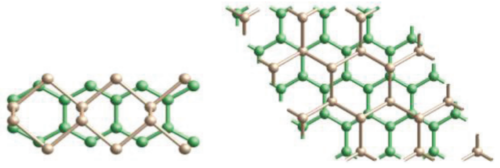

(a) (b)

**FIGURE 1.** The heterostructures of (a) black-P/graphene and (b) blue-P/ graphene. The green balls represent carbon while grey balls represent phosphorous atoms.

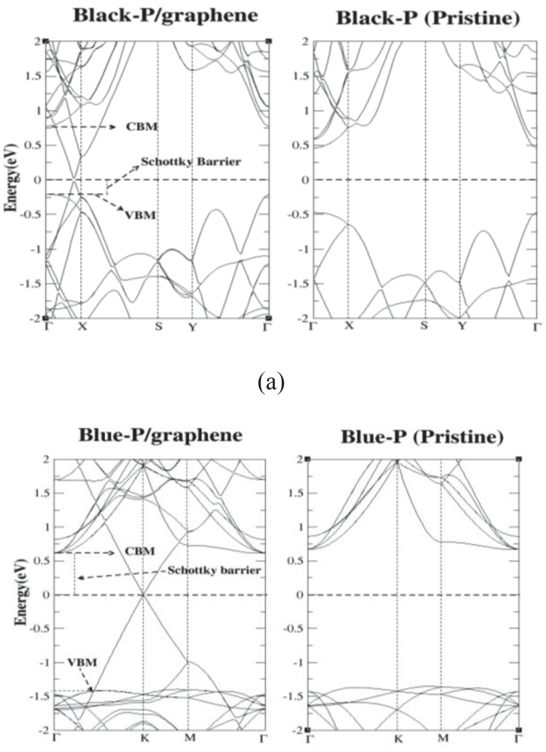
Figures 1(a) and 1(b) show the structures of black-P/graphene and blue-P/graphene heterolayers. In case of black-P/graphene heterostructure, supercell composed of 1×3 units of black-P and 1×4 units of graphene whereas blue-P/graphene heterostructure consists of 3×3 units of blue-P and 4×4 units of graphene. The above choice of supercell was opted to minimize the interfacial strain due to lattice mismatch. The strain induced in black-P/graphene and blue-P/graphene is less than 6% and 1%, respectively.

TABLE 1: Number of atoms (N), equilibrium separation between layers (d), binding energy (E) of bilayer structure and energy difference between the CBM and VBM (ΔE) with respect to pristine monolayers.

| | **Black-P/graphene** | **Blue-P/graphene** | **Monolayer black-P** | **Monolayer blue-P** |
|---|---|---|---|---|
| Number of atoms (N) | 28 | 50 | 12 | 18 |
| d (Å) | 3.63 | 3.63 | -- | -- |
| E (meV/atom) | 15.26 | 17.37 | -- | -- |
| ΔE (eV) | 0.98 | 2.03 | 0.92 | 2.04 |

The binding energy/atom of blue-P/graphene is found to be slightly greater than black-P/graphene suggesting blue-P/graphene heterostructure to be energetically favorable over black-P/graphene (Table 1). In the heterostructures of black-P/graphene and blue-P/graphene, the energy difference between valance band maxima (VBM) and conduction band minima (CBM) remain nearly same as that of the energy difference in the corresponding pristine monolayer counterpart (Table 1). Note that the energy differences between the VBM and CBM in heterostructures are taken with respect to the respective valance band and conduction band edges of the pristine monolayer in the heterostructures (Figure 2 (a) and 2(b)).

Moreover, the graphene induced well-known Dirac-cone character, which lies between Γ and X points in black-P/graphene and at K point in blue-P/graphene, is formed at the Fermi level ($E_F = 0$) (Figure 2.). All these observations along with a tiny splitting of ~ 0.03eV in black-P/graphene suggests that the features of pristine graphene and phosphorene are not much altered on formation of their heterojunction, indicating weak interaction between them. The order of magnitude of interlayer interaction energy is a few meV (Table 1), which suggests that the considered systems interact via weak van der waals forces.



(a)

(b)

**FIGURE 2.** The band-structures of (a) black-P/graphene and black-P pristine monolayer (b) blue-P/graphene and blue-P pristine monolayer.

In black-P/graphene the valance band edge that corresponds to monolayer black-P is closer to the Fermi level which indicates *p*-type character, whereas, in blue-P/graphene the corresponding conduction band edge of monolayer blue-P is closer to Fermi level, indicating *n*-type character, that results into the formation of Schottky barrier. Note that Schottky barrier is the excitation energy of electrons from graphene to phosphorene or vice-versa. For *p*-type materials, the Schottky barrier is defined as the difference between the Fermi level and the valance band edge and for *n*-type materials it is the difference between the conduction band edge and the Fermi level.

Now we apply an external electric field along z direction *i.e*, perpendicular to the phosphorene and graphene plane. Without any electric field, the Dirac point is formed at the Fermi level and therefore no charge transfer occurs between phosphorene and graphene in both heterostructures.

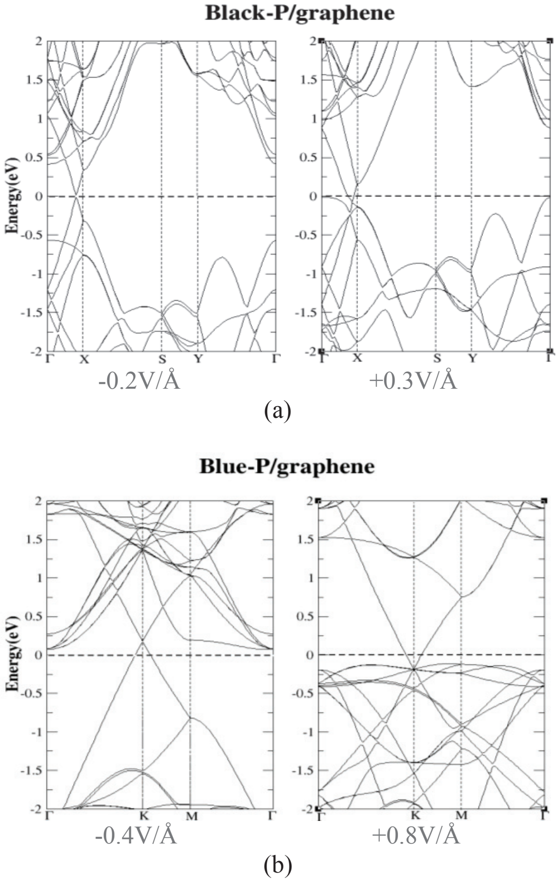


**FIGURE 3.** The effect of electric field on the band-structures of (a) black-P/graphene and (b) blue-P/graphene.

On applying an electric field > +0.2V/Å, the Dirac point moves within the valance band region on crossing the Fermi level thereby resulting into self-induced p-type doping in the black-P/graphene heterostructure. On the other hand, Dirac-point remain in contact with Fermi level on the application of negative electric field whereas the Schottky barrier keeps on increasing and this prevents the electron transfer from phosphorene to graphene.

In blue-P/graphene, the Dirac point moves above the CBM at an electric field of -0.4V/Å that results into so called n-type self induced doping in the heterostructure. On the other hand, positive field (+0.8V/Å) shifts the Dirac point in valance band region below Fermi energy, thereby, resulting into p-type self induced doping effect. These finding are very crucial for the van der waal hetero-structure based device fabrications.

## CONCLUSIONS

In the present work, DFT calculations have been performed to investigate the electronic properties of graphene based hetero-structures of black and blue phosphorene. The Dirac cone of graphene gets induced in the heterostructure of graphene with both black-P and blue-P. Dirac cone in heterostructures show tunabilty with external electric field that results into so called self induced p-type or n-type doping effect. All these features may prove useful in fabrication of devices based on Van der waal heterojunctions.

## ACKNOWLEDGMENTS

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